Yu-Shan Lin

Department of Chemistry
Tufts University
62 Talbot Avenue
Medford, MA 02155

Tel: (617)627-3689
Email: yu-shan.lin@tufts.edu
http://ase.tufts.edu/chemistry/lin/index.html

APPOINTMENT

Associate Professor, Department of Chemistry, Tufts University, 2018–present

Assistant Professor, Department of Chemistry, Tufts University, 2012–2018

EDUCATION

Bio-X Postdoctoral Fellow, Department of Chemistry, Stanford University, 2009–2012
Advisor: Professor Vijay S. Pande

Ph.D., Chemistry, University of Wisconsin–Madison, 2009
Thesis title: Theoretical vibrational spectroscopy of water and peptides
Advisor: Professor James L. Skinner

M.S., Chemistry, University of Wisconsin–Madison, 2007
Advisor: Professor James L. Skinner

B.S., Chemistry, National Taiwan University, 2004
Advisor: Professor Pi-Tai Chou

SELECTED FELLOWSHIPS AND AWARDS

- Faculty Achievement Award, Department of Chemistry, Tufts University, 2023
- Hirschfelder Visitor, University of Wisconsin–Madison, 2023
- Rising Innovator Award, Tufts University, 2023
- Annual Women Leadership Award, Rotary Club of Cambridge, 2023
- Machine Learning in the Chemical Sciences & Engineering Award, Camille and Henry Dreyfus Foundation, 2020
- ACS OpenEye Outstanding Junior Faculty Award in Computational Chemistry, American Chemical Society, 2015

CURRENT FUNDING

- 2R01GM124160 (PI: Lin) 2023/9/20–2027/6/30
  NIH/NIGMS $1,279,244 (total award)
  Understanding and designing cyclic peptides
- Beckman Scholars Program (Director: Lin) 2023/6/1–2026/8/31
  Arnold and Mabel Beckman Foundation $156,000
- Program for Machine Learning in the Chemical Sciences & Engineering (PI: Lin)
  Camille and Henry Dreyfus Foundation $120,000 (total award)

Low-supervision machine learning for automated analysis of molecular dynamics simulations

- R01AI168166 (PI: Shoulders) 2022/9/19–2027/7/31
  NIH/NIAID $311,944 (total subaward)
  Defining the interplay between viral adaptation and host proteostasis

PUBLICATIONS

- J. Damjanovic, **Y.-S. Lin**, J. M. Murphy, "Modeling changes in molecular dynamics time series as Wasserstein barycentric interpolations," *2023 International Conference on Sampling Theory and Applications (SampTA)*, New Haven, CT, USA, July 10–14, 2023; IEEE Xplore, accepted.
- J. Y. K. Wong, A. I. Ekanayake, S. Kirberger, R. Qiu, A. I. Ekanayake, P. Kelich, S. Sarkar, J. Li, K. X. Fernandez, E. R. Alvizo-Paez, J. Miao, S. Kalhor-Monfared, J. J. Dwyer, H. Kang, H. Choi, J. M. Nuss, J. C. Vederas, **Y.-S. Lin**, M. S. Macauley, L. Vukovic, W. Pomerantz, R. Derda, "Genetically-encoded discovery of perfluoroaryl-macrocycles that bind to albumin and exhibit extended circulation in-vivo," *Nat. Commun.* **14**, 5654 (2023).
- T. Hui,† M. L. Descoteaux,† J. Miao,† **Y.-S. Lin**, "Training neural network models using molecular dynamics simulation results to efficiently predict cyclic hexapeptide structural ensembles," *J. Chem. Theory Comput.* **19**, 4757 (2023).
  † Equal contributions.
- J. M. Mortensen,† J. Damjanovic,† J. Miao, T. Hui, **Y.-S. Lin**, "A backbone-dependent rotamer library with high (ϕ, ψ) coverage using metadynamics simulations," *Protein Sci.* **31**, e4491 (2022).
  † Equal contributions.
- X. Ye, Y.-C. Lee, Z. Gates, Y. Ling, J. Mortensen, F.-S. Yang, **Y.-S. Lin**, B. L. Pentelute, "Binary combinatorial scanning reveals potent poly-alanine-substituted inhibitors of protein–protein interactions," *Comm. Chem.* **5**, 128 (2022).
- J. Yoon, E. E. Nekongo, J. E. Patrick, T. Hui, A. M. Phillips, A. I. Ponomarenko, S. J. Hendel, R. M. Sebastian, Y. M. Zhang, V. L. Butty, C. B. Ogbunugafor, **Y.-S. Lin**, M. D. Shoulders, "The host cell's endoplasmic reticulum proteostasis network profoundly shapes the protein sequence space accessible to HIV envelope," *PLOS Biol.* **20**, e3001569 (2022).
- J. Miao, M. Descoteaux, **Y.-S. Lin**, "Structure prediction of cyclic peptides by molecular dynamics + machine learning," *Chem. Sci.* **12**, 14927–14936 (2021).
- J. Damjanovic, J. Murphy,* **Y.-S. Lin**,* "CATBOSS: Cluster analysis of trajectories based on segment splitting," *J. Chem. Inf. Model.* **61**, 5066–5081 (2021).
  *Co-corresponding authors.
- J. Damjanovic,† J. Miao,† H. Huang,† **Y.-S. Lin**, "Elucidating solution structures of cyclic peptides using molecular dynamics simulation," *Chem. Rev.* **121**, 2292–2324 (2021).
  † Equal contributions.
- H. Huang,† J. Damjanovic,† J. Miao, **Y.-S. Lin**, "Cyclic peptides: Backbone rigidification and capability of mimicking motifs at protein–protein interfaces," *Phys. Chem. Chem. Phys.* **23**, 607–616 (2021).
  † Equal contributions.
- K. Makwana, M. Sarnowski, J. Miao, **Y.-S. Lin**, J. Del Valle, "From aggregation to inhibition: N-amination converts amyloidogenic tau peptides into soluble antagonists of cellular seeding," *ACS Chem. Neurosci.* **12**, 3928–3938 (2021).

- J. Pace, C. Abakah, A. Moyer, J. Miao, K. Deprey, R. Cerulli, **Y.-S. Lin**, J. Baleja, D. Baker, J. Kritzer, "Stapled beta-hairpins using 4-mercaptoproline," *J. Am. Chem. Soc.* **143**, 15039–15044 (2021).
- J. Y.-K. Wong, R. Mukherjee, J. Miao, O. Bilyk, V. Triana, M. Miskolzie, A. Henninot, J. J. Dwyer, A. Iampolska, S. Kharchenko, D. Voluchnyuk, **Y.-S. Lin**, L.-M. Postovit, R. Derda, "Genetically-encoded discovery of proteolytically stable bicyclic inhibitors for morphogen NODAL," *Chem. Sci.* **12**, 9694–9703 (2021).
- T. Balema, J. Miao, N. Wasio, C. Murphy, A. Larson, D. Patel, **Y.-S. Lin**,* E. C. Sykes,* "Visualizing and understanding ordered surface phases during the Ullmann coupling reaction" *J. Phys. Chem. C* **125**, 7675–7685 (2021).
  *Co-corresponding authors.
- A. E. Cummings,† J. Miao,† D. P. Slough, S. M. McHugh, J. A. Kritzer,* **Y.-S. Lin**,* "Beta-branched amino acids stabilize specific conformations of cyclic hexapeptides," *Biophys. J.* **116**, 433–444 (2019).
  † Equal contributions. *Co-corresponding authors.
- E. A. Chen and **Y.-S. Lin**, "Using synthetic peptides and recombinant collagen to understand DDR-collagen interactions," *Biochim. Biophys. Acta Mol. Cell Res.* **1866**, 118458 (2019).
- T. Balema, N. Ulumuddin, C. Murphy, D. Slough, Z. Smith, R. Hannagan, N. Wasio, A. Larson, D. Patel, K. Groden, J.-S. McEwen,* **Y.-S. Lin**,* E. C. Sykes,* "Controlling molecular switching via chemical functionality; ethyl vs. methoxy rotors," *J. Phys. Chem. C* **123**, 23738–23746 (2019).
  *Co-corresponding authors.
- C. Tobon, L. C. Palacio, B. Chidipi, D. P. Slough, T. Tran, N. Tran, M. Reiser, **Y.-S. Lin**, B. Herweg, D. Sayad, J. Saiz, S. Noujaim, "The antimalarial chloroquine reduces the burden of persistent atrial fibrillation," *Front. Pharmacol.* **10**, 1392 (2019).
- D. P. Slough,† S. M. McHugh,† A. E. Cummings, P. Dai, B. L. Pentelute, J. A. Kritzer, **Y.-S. Lin**, "Designing well-structured cyclic pentapeptides based on sequence–structure relationships," *J. Phys. Chem. B* **122**, 3908–3919 (2018).
  † Equal contributions.
- D. P. Slough,† S. M. McHugh,† **Y.-S. Lin**, "Understanding and designing head-to-tail cyclic peptides," *Biopolymers* **109**, e23113 (2018).
  † Equal contributions.
- A. Mekkat,† E. Poppleton,† B. An, R. Visse, H. Nagase, D. L. Kaplan, B. Brodsky,* **Y.-S. Lin**,* "Effects of flexibility of the $\alpha 2$ chain of type I collagen on collagenase cleavage," *J. Struct. Biol.* **203**, 247–254 (2018).
  † Equal contributions. *Co-corresponding authors.
- Y. Qiu, A. Mekkat, H. Yu, S. Yigit, S. Hamaia, R. W. Farndale, D. L. Kaplan, **Y.-S. Lin**,* B. Brodsky,* "Collagen Gly missense mutations: Effect of residue identity on collagen structure and integrin binding," *J. Struct. Biol.* **203**, 255–262 (2018).
  *Co-corresponding authors.
- Y. Qiu, E. Poppleton, A. Mekkat, H. Yu, S. Banerjee, S. E. Wiley, J. E. Dixon, D. L. Kaplan, **Y-S. Lin**, and B. Brodsky "Enzymatic phosphorylation of Ser in a type I collagen peptide," *Biophys. J.* **115**, 2327–2335 (2018).
- A. M. Phillips, A. I. Ponomarenko, K. Chen, O. Ashenberg, J. Miao, S. M. McHugh, V. L. Butty, C. A. Whittaker, C. L. Moore, J. D. Bloom, **Y.-S. Lin**, M. D. Shoulders, "Destabilized adaptive influenza variants critical for innate immune system escape are potentiated by host chaperones," *PLOS Biol.* **17**, e3000008 (2018).

- A. M. Phillips, M. B. Doud, L. O. Gonzalez, V. L. Butty, **Y.-S. Lin**, J. D. Bloom, M. D. Shoulders, "Enhanced ER proteostasis and temperature differentially impact the mutational tolerance of influenza hemagglutinin," *eLife* **7**, e38795 (2018).
- M. Jafari, H. Yu, J. Wickware, **Y.-S. Lin**, R. Derda, "Light-responsive bicyclic peptides," *Org. Biomol. Chem.* **16**, 7588–7594 (2018).
- Y. Takemoto,† D. P. Slough,† G. Meinke, C. Katnik, Z. A. Graziano, M. M. Alhadidy, M. Reiser, C. Bujjibabou, R. Ramirez, O. Salvador-Montanes, S. Ennis, G. Gurrero, M. Haburcak, C. Diehl, J. Cuevas, J. Jalife, A. Bohm, **Y.-S. Lin**, S. F. Noujaim, "Structural basis for the antiarrhythmic blockade of a potassium channel with a small molecule," *FASEB J.* **32**, 1778–1793 (2018).
  † Equal contributions.
- J. R. Rogers, S. M. McHugh, **Y.-S. Lin**, "Predictions for α-helical glycopeptide design from structural bioinformatics analysis," *J. Chem. Inf. Model.* **57**, 2598–2611 (2017).
- D. P. Slough, H. Yu, S. M. McHugh, **Y.-S. Lin**, "Toward accurately modeling *N*-methylated cyclic peptides," *Phys. Chem. Chem. Phys.* **19**, 5377–5388 (2017).
- S. M. McHugh,† H. Yu,† D. P. Slough, **Y.-S. Lin**, "Mapping the sequence–structure relationships of simple cyclic hexapeptides," *Phys. Chem. Chem. Phys.* **19**, 3315–3324 (2017).
  †Equal contributions.
- N. A. Wasio, D. P. Slough, Z. C. Smith, C. J. Ivimey, S. W. Thomas III, **Y.-S. Lin**,* E. C. H. Sykes,* "Correlated rotational switching in 2D self-assembled molecular rotor arrays," *Nat. Comm.* **8**, 16057 (2017).
  *Co-corresponding authors.
- Y. Li, N. P. Lavey, J. A. Coker, J. E. Knobbe, D. C. Truong, H. Yu, **Y.-S. Lin**, S. L. Nimmo, A. S. Duerfeldt, "Consequences of depsipeptide substitution on the ClpP activation activity of antibacterial acyldepsipeptides," *ACS Med. Chem. Lett.* **8**, 1171–1176 (2017).
- S. Mong, F. Cochran, H. Yu, Z. A. Graziano, **Y.-S. Lin**, J. R. Cochran, B. L. Pentelute, "Heterochiral knottin protein: Folding and solution structure," *Biochemistry* **56**, 5720–5725 (2017).
- A. M. Phillips, L. O. Gonzalez, E. E. Nekongo, A. I. Ponomarenko, S. M. McHugh, V. Butty, S. S. Levine, **Y.-S. Lin**, L. A. Mirny, M. D. Shoulders, "Host proteostasis modulates influenza evolution," *eLife* **6**, e28652 (2017).
- L. Peraro, Z. Zou, K. M. Makwana, A. E. Cummings, H. L. Ball, H. Yu, **Y.-S. Lin**, B. Levine, J. Kritzer, "Diversity-oriented stapling yields intrinsically cell-penetrant inducers of autophagy," *J. Am. Chem. Soc.* **139**, 7792–7802 (2017).
- S. M. McHugh,† J. R. Rogers,† H. Yu, **Y.-S. Lin**, "Insights into how cyclic peptides switch conformations," *J. Chem. Theory Comput.* **12**, 2480–2488 (2016).
  †Equal contributions.
- S. M. McHugh,† J. R. Rogers,† S. A. Solomon,† H. Yu,† **Y.-S. Lin**, "Computational methods to design cyclic peptides," *Curr. Opin. Chem. Biol.* **34**, 95–102 (2016).
  †Equal contributions.
- P. Chhum,† H. Yu,† B. An, B. Doyon, **Y.-S. Lin**,* B. Brodsky,* "Consequences of glycine mutations in the fibronectin binding sequence of collagen," *J. Biol. Chem.* **291**, 27073–27086 (2016).
  †Equal contributions. *Co-corresponding authors.
- S. Yigit,† H. Yu,† B. An, S. Hamaia, R. W. Farndale, D. L. Kaplan, **Y.-S. Lin**,* B. Brodsky,* "Mapping the effect of Gly mutations in collagen on $\alpha 2\beta 1$ integrin binding," *J. Biol. Chem.* **291**, 19196–19207 (2016).
  †Equal contributions. *Co-corresponding authors.

- M. D. Simon, Y. Maki, A. A. Vinogradov, C. Zhang, H. Yu, **Y.-S. Lin**, Y. Kajihara, B. L. Pentelute, "D-Amino acid scan of two small proteins," *J. Am. Chem. Soc.* **138**, 12099–12111 (2016).
- B. An, **Y.-S. Lin**, B. Brodsky, "Collagen interactions: Drug design and delivery," *Adv. Drug Deliv. Rev.* **97**, 69–84 (2016).
- H. Yu and **Y.-S. Lin**, "Toward structure prediction of cyclic peptides," *Phys. Chem. Chem. Phys.* **17**, 4210–4219 (2015).
- J. S. Quartararo, M. R. Eshelman, L. Peraro, H. Yu, J. D. Baleja, **Y.-S. Lin**, J. A. Kritzer, "A bicyclic peptide scaffold promotes phosphotyrosine mimicry and cellular uptake," *Bioorg. Med. Chem.* **22**, 6387–6319 (2014).
- Y. Zou, A. M. Spokoyny, C. Zhang, M. D. Simon, H. Yu, **Y.-S. Lin**, B. L. Pentelute, "Convergent diversity-oriented side-chain macrocyclization scan for unprotected polypeptides," *Org. Biomol. Chem.* **12**, 566–573 (2014).
- A. M. Spokoyny, Y. Zou, J. J. Ling, H. Yu, **Y.-S. Lin**, B. L. Pentelute, "A perfluoroaryl-cysteine S_NAr chemistry approach to unprotected peptide stapling," *J. Am. Chem. Soc.* **135**, 5946–5949 (2013).
- C. R. Baiz, **Y.-S. Lin**, C. S. Peng, K. A. Beauchamp, V. A. Voelz, V. S. Pande, A. Tokmakoff, "A molecular interpretation of 2D IR protein folding experiments with Markov state models," *Biophys. J.* **106**, 1359–1370 (2014).
- **Y.-S. Lin** and V. S. Pande, "Effects of familial mutations on the monomer structure of Aβ_{42}," *Biophys. J.* **103**, L47–L49 (2012).
- K. A. Beauchamp, R. McGibbon, **Y.-S. Lin**, V. S. Pande, "Simple few-state models reveal hidden complexity in protein folding," *Proc. Natl. Acad. Sci. U.S.A.* **109**, 17807–17813 (2012).
- K. A. Beauchamp, **Y.-S. Lin**, R. Das, V. S. Pande, "Are protein force fields getting better? A systematic benchmark on 524 diverse NMR measurements," *J. Chem. Theory Comput.* **8**, 1409–1414 (2012).
- **Y.-S. Lin**, G. R. Bowman, K. A. Beauchamp, V. S. Pande, "Investigating how peptide length and a pathogenic mutation modify the structural ensemble of amyloid beta monomer," *Biophys. J.* **102**, 315–324 (2012).
- C. J. Tainter, P. A. Pieniazek, **Y.-S. Lin**, J. L. Skinner, "Robust three-body water simulation model," *J. Chem. Phys.* **134**, 184501 (2011).
- **Y.-S. Lin**, P. A. Pieniazek, M. Yang, J. L. Skinner, "On the calculation of rotational anisotropy decay, as measured by ultrafast polarization-resolved pump-probe experiments," *J. Chem. Phys.* **132**, 174505 (2010).
- A. M. Woys, **Y.-S. Lin**, A. S. Reddy, J. J. de Pablo, J. L. Skinner, M. T. Zanni, "2D IR lineshapes probe ovispirin peptide conformation and depth in lipid bilayers," *J. Am. Chem. Soc.* **132**, 2832–2838 (2010).
- A. S. Reddy, L. Wang, **Y.-S. Lin**, Y. L. Ling, M. T. Zanni, J. L. Skinner, J. J. de Pablo, "Solution structures of rat amylin peptide: Simulation, theory, and experiment," *Biophys. J.* **98**, 443–451 (2010).
- P. A. Pieniazek, **Y.-S. Lin**, J. L. Skinner, "Vibrational spectroscopy and dynamics of water confined inside reverse micelles," *J. Phys. Chem. B* **113**, 15017–15028 (2009).
- **Y.-S. Lin**, B. M. Auer, J. L. Skinner, "Water structure, dynamics, and vibrational spectroscopy in sodium bromide solutions," *J. Chem. Phys.* **131**, 144511 (2009).
- J. Manor, P. Mukherjee, **Y.-S. Lin**, H. Leonov, J. L. Skinner, M. T. Zanni, I. T. Arkin, "Gating mechanism of the influenza A M2 channel revealed by 1D and 2D IR spectroscopies," *Structure* **17**, 247 (2009).

- **Y.-S. Lin**, J. M. Shorb, P. Mukherjee, M. T. Zanni, J. L. Skinner, "Empirical amide I vibrational frequency map: Applications to isotope-edited membrane peptide bundles," *J. Phys. Chem. B* **113**, 592–602 (2009).
- J. L. Skinner, B. M. Auer, **Y.-S. Lin**, "Vibrational line shapes and spectral diffusion in liquid water," *Adv. Chem. Phys.* **142**, 59–103 (2009).
- D. E. Moilanen, E. E. Fenn, **Y.-S. Lin**, J. L. Skinner, B. Bagchi, M. D. Fayer, "Water inertial reorientation: Hydrogen bond strength and the angular potential," *Proc. Natl. Acad. Sci. U.S.A.* **105**, 5295–5300 (2008).
- **Y.-S. Lin**, S. G. Ramesh, J. M. Shorb, E. L. Sibert III, J. L. Skinner, "Vibrational energy relaxation of the bend fundamental of dilute water in liquid chloroform and *d*-chloroform," *J. Phys. Chem. B* **112**, 390–398 (2008).
- K.-C. Wu, **Y.-S. Lin**, Y.-S. Yeh, C.-Y. Chen, M. O. Ahmed, P.-T. Chou, Y.-S. Hon, "Design and synthesis of intramolecular hydrogen bonding systems. Their application in metal cation sensing based on excited state proton transfer reaction," *Tetrahedron* **60**, 11861–11868 (2004).
- K.-C. Wu, Y.-M. Cheng, **Y.-S. Lin**, Y.-S. Yeh, S.-C. Pu, Y.-H. Hu, J.-K. Yu, P.-T. Chou, "Competitive intramolecular hydrogen bonding formation and excited-state proton transfer reaction in 1-[(diethylamino)-methyl]-2-hydroxy-3-naphthaldehyde," *Chem. Phys. Lett.* **384**, 203–209 (2004).

SELECTED INVITED ORAL PRESENTATIONS

- University of Wisconsin–Madison, Theoretical Chemistry Institute Seminar, October 24, 2023
- 13th International Peptide Symposium, Brisbane, Australia, October 15–20, 2023
- Peptide Therapeutics Forum 2023, Basel, Switzerland, September 4–5, 2023
- Institute of Atomic and Molecular Sciences, Academia Sinica, Taipei, Taiwan, August 24, 2023
- Ewha Womans University, Chemistry Departmental Seminar, Seoul, Korea, August 18, 2023
- International Conference on Biological Physics 2023, Seoul, Korea, August 14–18, 2023
- American Chemical Society National Meeting, San Francisco, August 13–17, 2023
- New York University, Simons Center for Computational Physical Chemistry, March 20, 2023
- Asia Pacific Conference of Theoretical and Computational Chemistry, Quy Nhon, Vietnam, February 19–23, 2023
- Gordon Research Conference: Chemistry and Biology of Peptides, Oxnard CA, October 30–November 4, 2022
- Amber Developers Meeting, Tampa FL, June 2–4, 2022
- Vanderbilt University, Chemistry Departmental Seminar, April 11, 2022
- SUNY Binghamton, Chemistry Departmental Seminar, March 25, 2022
- Georgia Institute of Technology, Special Seminar, February 24, 2022
- American Peptide Society, e-Seminar, October 15, 2021
- Advancing Chemical and Materials Science through Machine Learning, Hariri Institute for Computing, Boston University, June 14, 2021
- Molecular Biophysics in the Northeast, Boston, November 9, 2019
- Boston Taiwanese Biotechnology Association Seminar Series, Cambridge, June 30, 2019
- Free Energy Calculations: Entering the Fourth Decade of Adventure in Chemistry and Biophysics, Santa Fe, June 16–21, 2019

- Stonehill College, Chemistry Departmental Seminar, November 30, 2018
- The Greater Boston Area Theoretical Chemistry Lecture Series (THEOCHEM), September 19, 2018
- Annual Meeting of the Biophysical Society of Canada, Montréal, Québec, May 24–26, 2017
- University of Washington–Seattle, Physical Chemistry Seminar, May 24, 2017
- University of California–Santa Barbara, Biomolecular Science and Engineering Seminar, May 17, 2017
- University of California–Merced, Chemistry and Chemical Biology Seminar, April 28, 2017
- University of Notre Dame, Physical/Analytical Chemistry Seminar, April 20, 2017
- Purdue University, Physical Chemistry Seminar, April 19, 2017
- American Chemical Society National Meeting, San Francisco, April 2–6, 2017
- University of Illinois at Urbana–Champaign, Chemical and Biomolecular Engineering Seminar, March 30, 2017
- Rutgers University, Proteomics/IQB@R and CABM Seminars, March 22, 2017
- Louisiana State University, LaCNS and Physical Chemistry Seminar, February 21, 2017
- Massachusetts Institute of Technology, Biophysics Seminar Series, February 8, 2017
- Trinity University, Chemistry Departmental Seminar, December 1, 2016
- Temple University, Chemistry Departmental Seminar, November 3, 2016
- Brigham Young University, Chemistry Departmental Seminar, March 25, 2016
- Boston College, Chemistry Departmental Seminar, March 22, 2016
- American Chemical Society National Meeting, San Diego, March 13–17, 2016
- Colby College, Chemistry Departmental Seminar, October 30, 2015
- University of Wisconsin–Madison, Theoretical Chemistry Institute Seminar, April 20, 2015
- Boston University, Physical Chemistry Seminar, November 19, 2014
- American Conference on Theoretical Chemistry, Telluride, July 20–24, 2014
- American Chemical Society National Meeting, New Orleans, April 7–11, 2013

TEACHING AT TUFTS

- Chemistry 1: Chemical Fundamentals
  First-semester general chemistry with up to 180 students (SP14, SP16, SP18)
- Chemistry 31: Physical Chemistry I
  Classical thermodynamics and statistical thermodynamics for science and engineering majors (FA15, FA20, FA22)
- Chemistry 32: Physical Chemistry II
  Quantum mechanics for science and engineering majors (SP20)
- Chemistry 133: Quantum Mechanics
  Upper and graduate-level quantum mechanics (FA12, FA13, FA23)
- Chemistry 135: Biophysical Chemistry
  Upper and graduate level biophysical chemistry (FA16, SP19, FA19, SP21, SP22, SP23)
- Chemistry 194: Computational Chemistry
  Special topic course with a hands-on curriculum on programming and molecular dynamics simulations (SP17)

PROFESSIONAL SERVICE

Editorial Advisory Board

- Peptide Science

Associate Editor

- Biochemistry

Peer Review

- Assorted journals, including *Chem. Sci.*, *J. Chem. Inf. Model.*, *J. Chem. Phys.*, *J. Chem. Theory Comput.*, *J. Med. Chem.*, *J. Phys. Chem. B*, *Nat. Biomed. Eng.*, *Nat. Chem.*, *Nat. Chem. Biol.*, *Org. Lett.*, *Phys. Chem. Chem. Phys.*, *PLOS Comp. Biol.*, *RSC Advances*, and *Science*.
- Grant proposals: American Chemical Society, Beckman Foundation, National Institutes of Health, and National Science Foundation.

Departmental Committees

- Computer Resources Committee, 2019–present
  (Committee chair 2019–present)
- Faculty Search Committee, 2012–2013, 2019–2020, 2022–2023
  (Committee chair 2022–2023)
- Undergraduate Studies Committee, 2022 spring
  (Committee chair 2022 spring)
- Student Awards Committee, 2014–2020, 2022 spring
  (Committee chair 2022 spring)
- Graduate Committee, 2012–2017, 2020–2022
  Coordinate the graduate program; recruit and admit graduate students; advise graduate students prior to their selection of a research advisor; monitor graduate student progress, especially the timely completion of degree requirements.
- Diversity, Equity, and Inclusion Committee, 2020–2021
  (Committee chair 2020–2021)
- Seminar Committee, 2016–2020
  (Committee chair 2018–2020)

School and University Committees

- Budget and University Priorities (elected), 2020–2025
  (Committee chair 2022–present)
- Research Storage Working Group, 2023–present
- Beckman Scholars Program at Tufts, 2022–present
  (Program director 2022–present)
- Committee on Faculty Work/Life, 2019–2020
- Information Technology Committee, 2015–2020

MENTORING AND ADVISING

Current Research Associate

- Dr. Jiayuan Miao, 2023–present

Current Postdoctoral Scholars

- Dr. Arghya Ghosh, 2022–present

- Dr. Maxim Secor, 2023–present

Current Graduate Students

- Francini Fonseca, 2017–present
- Tiffani Hui, 2020–present
- Nomindari Bayaraa, 2021–present
- Minh Ho, 2021–present

Group Alumni

- Marc Descoteaux, 2021–2023 (junior–master's)
  Marc was a 2021 Summer Scholar at Tufts.
  Marc is currently a graduate student in Materials Science and Mechanical Engineering at Harvard.
- Dr. Jovan Damjanovic, 2018–2023
  Jovan is currently a senior data scientist at Novo Nordisk.
- Dr. Jennifer Mortensen, IRACDA postdoctoral scholar, 2020–2022
  Jennifer is currently a teaching assistant professor at Worcester Polytechnic Institute.
- Kevin Schult, 2019–2022 (sophomore–senior)
  Kevin was a 2020 Beckman Scholar at Tufts.
  Kevin is currently a graduate student in the Department of Chemistry at Harvard.
- Yingjie (Tim) Ling, 2018–2021 (sophomore–senior)
  Tim was a 2019 Laidlaw Scholar at Tufts.
  Tim is currently a master's student in the Department of Computer Science at Carnegie Mellon University.
- Stephanie Kearing, master's student, 2019–2020
  Steph is currently a scientific technical reviewer at Boston Analytical.
- Omeir Khan, undergraduate researcher, 2018–2020 (junior–senior)
  Omeir was a 2019 Summer Scholar at Tufts.
  Omeir is currently a graduate student in the Department of Chemistry at BU.
- Aidan Fike, undergraduate researcher, 2018–2020 (junior–senior)
  Aidan was a 2019 Beckman Scholar at Tufts.
  Aidan is currently a software engineer at Ab Initio Software.
- Dr. He (Agnes) Huang, postdoctoral scholar, 2018–2020
  Agnes is currently an application scientist at OpenEye Scientific Software.
- Eric Chen, undergraduate researcher, 2017–2019 (junior–senior)
  Eric was a 2018 Summer Scholar at Tufts.
  Eric is currently a graduate student in the Department of Chemistry at NYU.
- Steph Xu, undergraduate researcher, 2017–2019 (junior–senior)
  Steph is currently a software engineer at Microsoft.
- Arya Mekkat, undergraduate researcher, 2015–2018 (first-year–senior)
  Arya was a 2017 Summer Scholar at Tufts.
  Arya went on to medical school at BU. She is currently doing her medical residency at the Boston Medical Center.
- Dr. Diana Slough, graduate student, 2012–2018
  Diana is currently a senior investigator at Roivant Sciences.

- Dr. Sean McHugh, graduate student, 2012–2018
  Sean is currently an associate director for portfolio operations and launch management at Sanofi.
- Dan McKeen, 2016–2017 (sophomore)
- Mong Mary Touch, graduate student, 2016–2017
- Dr. Hongtao Yu, postdoctoral scholar, 2012–2017
  Hongtao is currently an applied scientist at Amazon Lab126.
- Zachary Graziano, undergraduate researcher, 2015–2016 (sophomore–junior)
  Zach was a 2016 Summer Scholar at Tufts.
  Zach is currently a senior software engineer at Appcues.
- Dr. Julia Rogers, undergraduate researcher, 2014–2016 (junior–senior)
  Julia was a 2015 Beckman Scholar at Tufts.
  Julia went on to the Department of Chemistry at UC Berkeley for graduate school. She is currently a postdoctoral researcher at Columbia University.
- Sarah Solomon, master student, 2014–2016
  Sarah is currently a senior associate scientist at Alnylam Pharmaceuticals.
- Diana Gooding, master student, 2014–2015
- Joshua Levy, undergraduate researcher, 2012–2014 (junior–senior)
  Josh is currently a graduate student in the Department of Engineering Sciences and Applied Mathematics at Northwestern University.
- Owen Martin, undergraduate researcher, 2013–2014 (first-year)
  Owen is currently a graduate student in the Department of Computer Science at University of Colorado, Boulder.
- Jordan Rossen, undergraduate researcher, 2013–2014 (first-year)
  Jordan is currently an associate computational biologist at the Broad Institute of MIT and Harvard.
- Andrew Rosen, undergraduate researcher, 2013–2014 (junior)
  Andrew was a 2014 Goldwater Scholar.
  Andrew is currently a graduate student in the Department of Chemical Engineering at Northwestern University.
- Benjamin Kim, undergraduate researcher, 2012–2013 (junior)